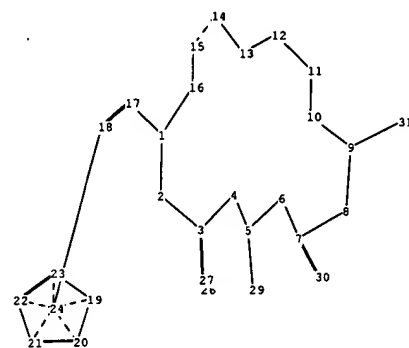
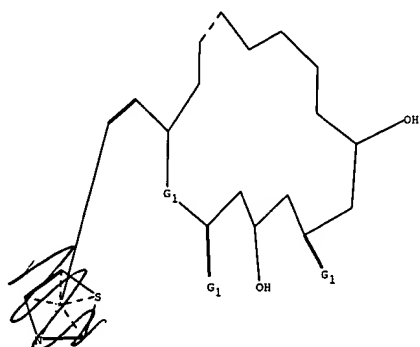


(Untitled)



chain nodes :

17 18 26 27 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 19 20 21 22 23

chain bonds :

1-17 3-27 5-29 7-30 9-31 17-18

ring bonds :

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
15-16 19-20 19-23 20-21 21-22 22-23

exact/norm bonds :

1-2 1-16 1-17 2-3 3-4 3-27 4-5 5-6 5-29 6-7 7-8 7-30 8-9 9-10 9-31 10-11
11-12 12-13 13-14 14-15 15-16 17-18 19-20 19-23 20-21 21-22 22-23

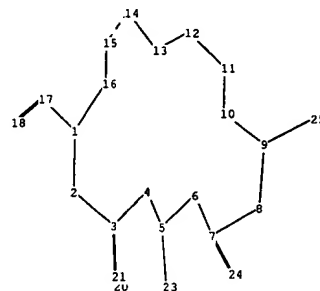
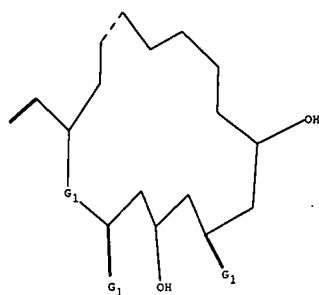
isolated ring systems :

containing 1 : 19 :

G1:O,S

Match level :

1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 31:CLASS



chain nodes :

17 18 20 21 23 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

chain bonds :

1-17 3-21 5-23 7-24 9-25 17-18

ring bonds :

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16

exact/norm bonds :

1-2 1-16 1-17 2-3 3-4 3-21 4-5 5-6 5-23 6-7 7-8 7-24 8-9 9-10 9-25 10-11 11-12 12-13 13-14 14-15 15-16 17-18

isolated ring systems :

containing 1 :

G1:O,S

Match level :

1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 20:CLASS 21:CLASS
23:CLASS 24:CLASS 25:CLASS

***** Welcome to STN International *****

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
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 NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
 NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
 NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
 NEWS 9 Jun 03 New e-mail delivery for search results now available
 NEWS 10 Jun 10 MEDLINE Reload
 NEWS 11 Jun 10 PCTFULL has been reloaded
 NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
 NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
 saved answer sets no longer valid
 NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
 NEWS 15 Jul 30 NETFIRST to be removed from STN
 NEWS 16 Aug 08 CANCERLIT reload
 NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
 NEWS 18 Aug 08 NTIS has been reloaded and enhanced
 NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
 now available on STN
 NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
 NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
 NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
 NEWS 23 Sep 03 JAPIO has been reloaded and enhanced

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
 CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
 AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
 NEWS HOURS STN Operating Hours Plus Help Desk Availability
 NEWS INTER General Internet Information
 NEWS LOGIN Welcome Banner and News Items
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN
 NEWS WWW CAS World Wide Web Site (general information)

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***** STN Columbus *****

FILE 'HOME' ENTERED AT 22:58:00 ON 08 SEP 2002

=> file reg
 COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
 FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 22:58:14 ON 08 SEP 2002
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 6 SEP 2002 HIGHEST RN 447682-31-7
 DICTIONARY FILE UPDATES: 6 SEP 2002 HIGHEST RN 447682-31-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

L1 STRUCTURE UPLOADED

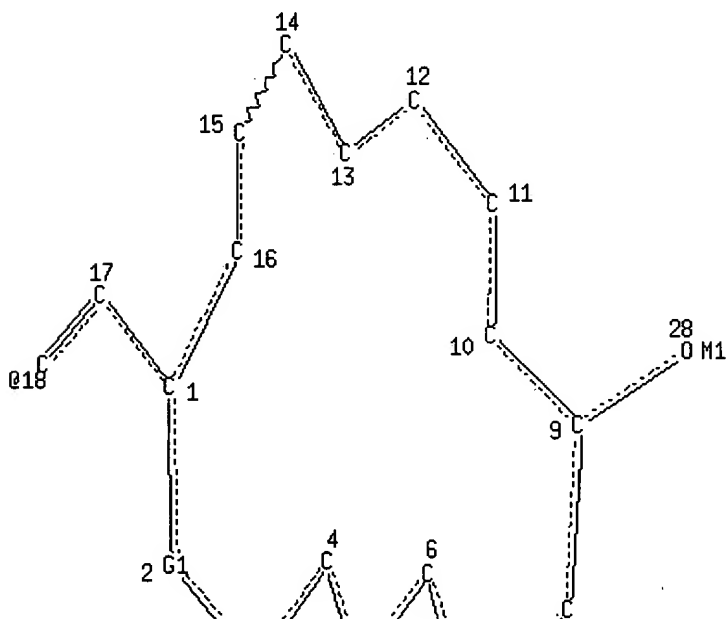
=> d 11

L1 HAS NO ANSWERS

L1 STR

0 29 S 30

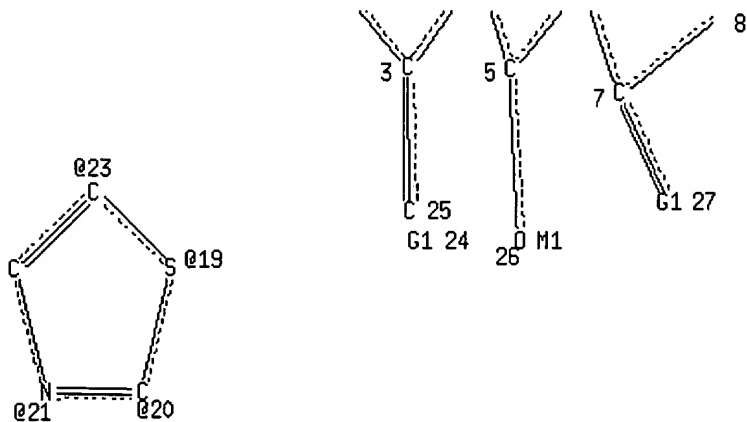
Page 1-A



Page 1-B

@22

Page 2-A



Page 2-B

VAR G1=29/30

VPA 18-19/20/21/22/23 S

NODE ATTRIBUTES:

HCOUNT	IS M1	AT	26
HCOUNT	IS M1	AT	28
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS C	AT	17
NSPEC	IS C	AT	18
NSPEC	IS R	AT	19
NSPEC	IS R	AT	20
NSPEC	IS R	AT	21
NSPEC	IS R	AT	22
NSPEC	IS R	AT	23
NSPEC	IS C	AT	24
NSPEC	IS C	AT	25
NSPEC	IS C	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28
DEFAULT MLEVEL IS ATOM			
MLEVEL IS CLASS AT 17 18 25 26 28 29 30			
DEFAULT ECLEVEL IS LIMITED			

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 23:04:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE

100.0% PROCESSED 7 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 7 TO 298

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 139.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 23:04:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 134 TO ITERATE

100.0% PROCESSED 134 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA SSS FUL L1

=>

L4 STRUCTURE UPLOADED

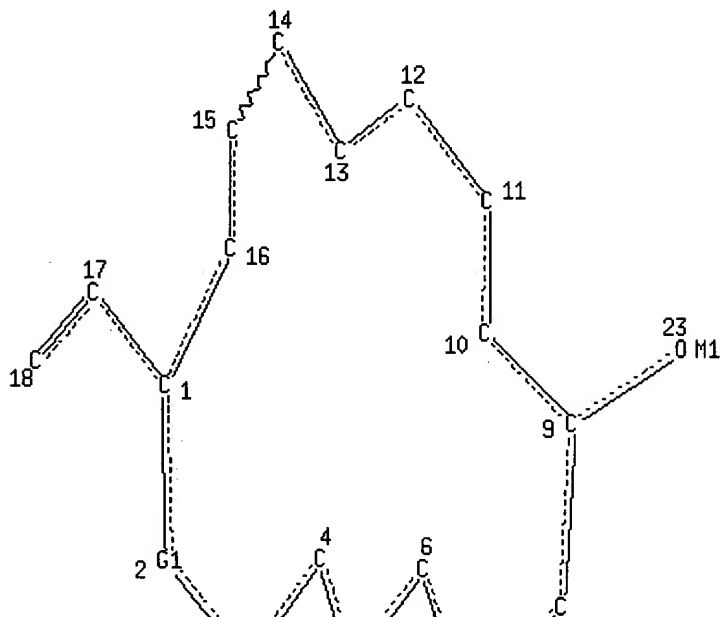
=> d 14

L4 HAS NO ANSWERS

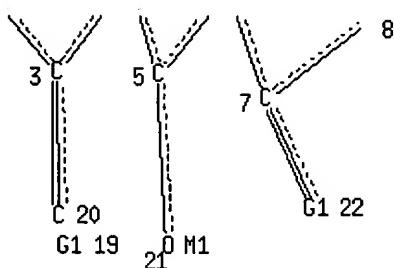
L4 STR

0 24 S 25

Page 1-A



Page 1-B



Page 2-B

VAR G1=24/25

NODE ATTRIBUTES:

HCOUNT	IS	M1	AT	21
HCOUNT	IS	M1	AT	23
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	R	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12

NSPEC IS R AT 13
 NSPEC IS R AT 14
 NSPEC IS R AT 15
 NSPEC IS R AT 16
 NSPEC IS C AT 17
 NSPEC IS C AT 18
 NSPEC IS C AT 19
 NSPEC IS C AT 20
 NSPEC IS C AT 21
 NSPEC IS C AT 22
 NSPEC IS C AT 23

DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 17 18 20 21 23 24 25
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

=> s 14

SAMPLE SEARCH INITIATED 23:05:53 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 1165 TO ITERATE

85.8% PROCESSED 1000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 21253 TO 25347
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

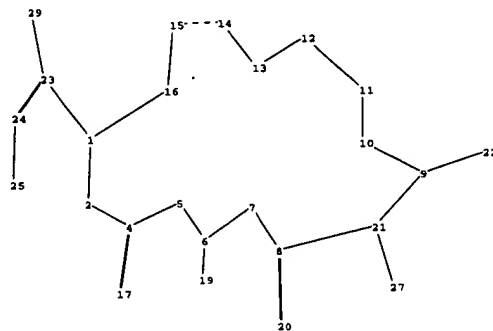
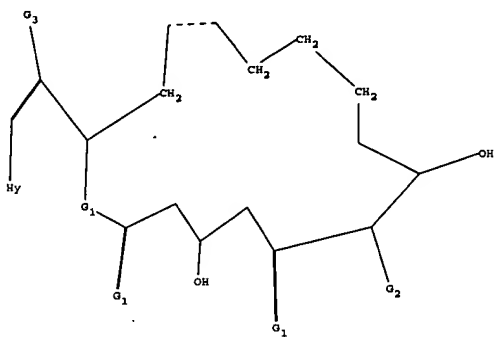
=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 139.90 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 23:06:05 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 22717 TO ITERATE

100.0% PROCESSED 22717 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>



chain nodes :

17 19 20 22 23 24 25 27 29

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21

chain bonds :

1-23 4-17 6-19 8-20 9-22 21-27 23-24 23-29 24-25

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15 15-16

exact/norm bonds :

1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 8-20 8-21 9-10 9-21 9-22 10-11 11-12 12-13 13-14 14-15 15-16 21-27 23-24 23-29 24-25

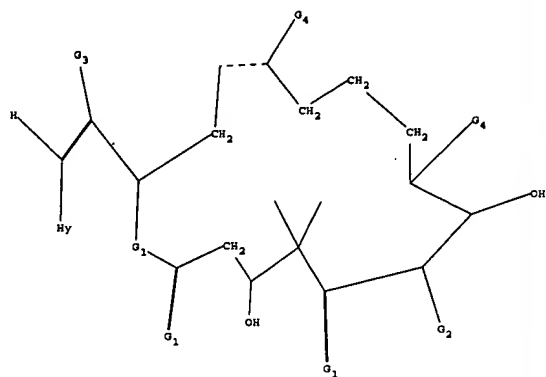
G1:O,S

G2:CH₃,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

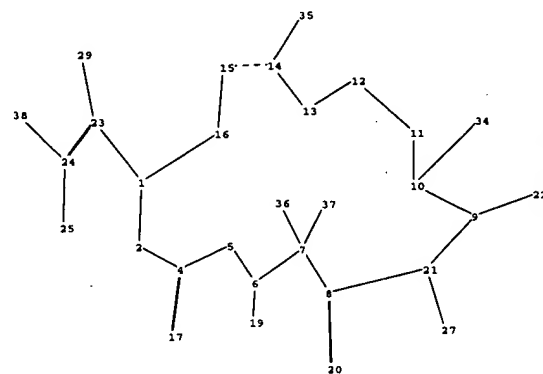
G3:H,Ak

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 25:Atom 27:CLASS 29:CLASS



e 1k
Ph



e 11
30

chain nodes :

17 19 20 22 23 24 25 27 29 30 31 34 35 36 37 38

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21

chain bonds :

1-23 4-17 6-19 7-37 7-36 8-20 9-22 10-34 14-35 21-27 23-24 23-29 24-25 24-38 30-31

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15 15-16

exact/norm bonds :

1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-37 7-36 8-20 8-21 9-10 9-21 9-22 10-11 10-34 11-12 12-13 13-14 14-15 14-35 15-16 21-27 23-24 23-29 24-25 24-38 30-31

G1:O,S

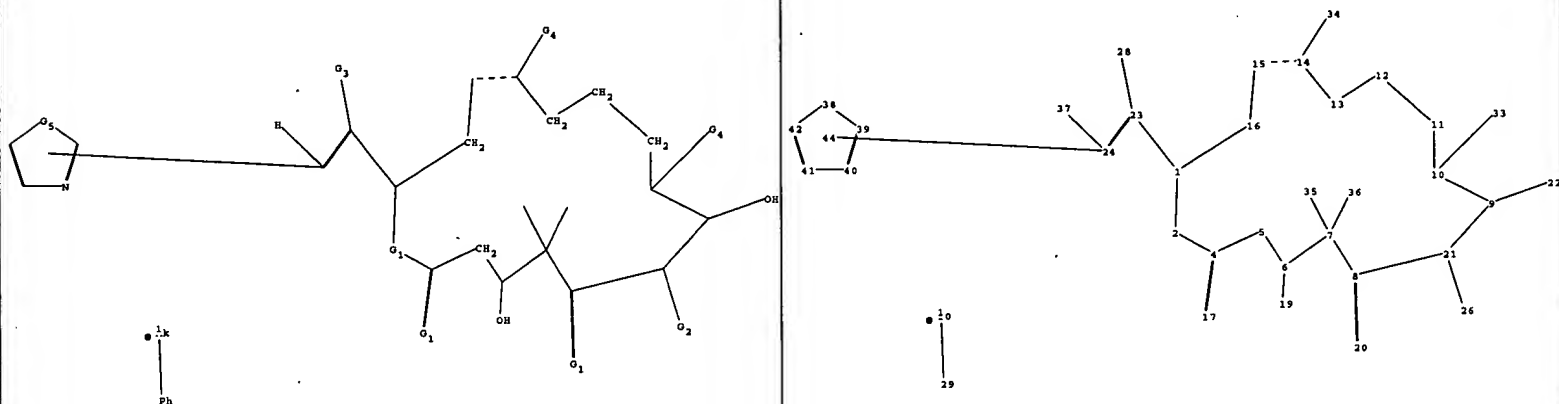
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

G4:Ph,Ak,H,[*1]

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 25:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS



chain nodes :

17 19 20 22 23 24 26 28 29 30 33 34 35 36 37

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21 38 39 40 41 42

chain bonds :

1-23 4-17 6-19 7-36 7-35 8-20 9-22 10-33 14-34 21-26 23-24 23-28 24-37 29-30

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
15-16 38-39 38-42 39-40 40-41 41-42

exact/norm bonds :

1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21
9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37
29-30 38-39 38-42 39-40 40-41 41-42

G1:O,S

G2:CH₃,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

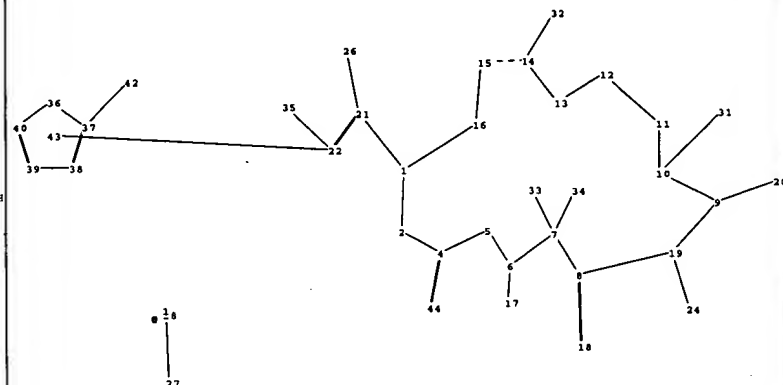
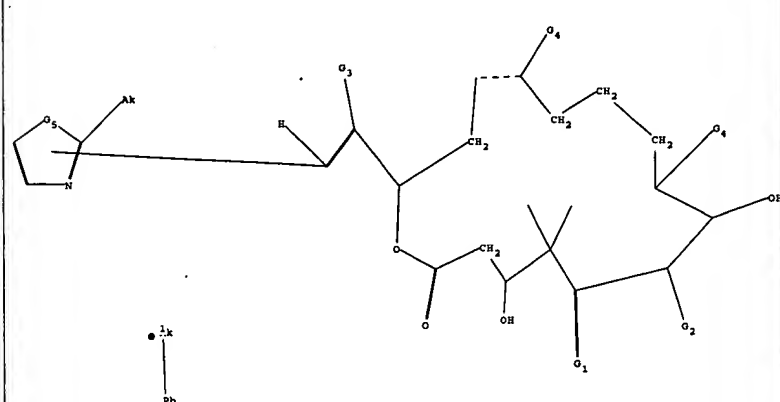
G3:H,Ak

G4:Ph,Ak,H,[*1]

G5:O,S

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 44:CLASS



chain nodes :

17 18 20 21 22 24 26 27 28 31 32 33 34 35 42 44

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 19 36 37 38 39 40

chain bonds :

1-21 4-44 6-17 7-34 7-33 8-18 9-20 10-31 14-32 19-24 21-22 21-26 22-35 27-28
37-42

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-19 9-10 9-19 10-11 11-12 12-13 13-14 14-15
15-16 36-37 36-40 37-38 38-39 39-40

exact/norm bonds :

1-2 1-16 1-21 2-4 4-5 4-44 5-6 6-7 6-17 7-8 7-34 7-33 8-18 8-19 9-10 9-19
9-20 10-11 10-31 11-12 12-13 13-14 14-15 14-32 15-16 19-24 21-22 21-26 22-35
27-28 36-37 36-40 37-38 37-42 38-39 39-40

G1:O,S

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

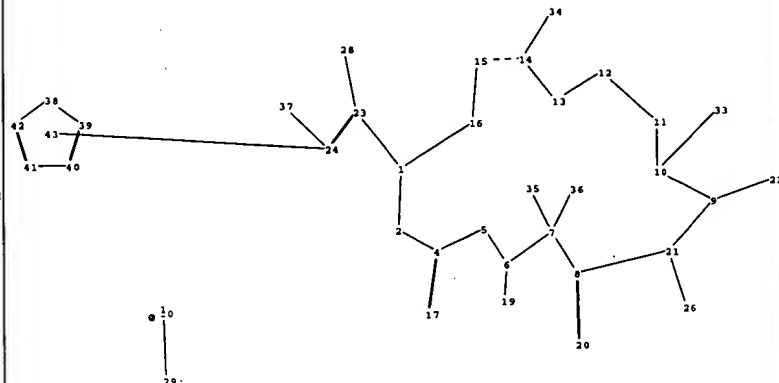
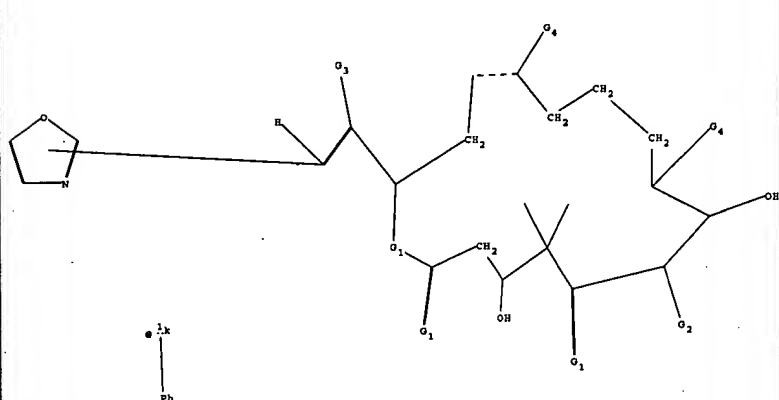
G3:H,Ak

G4:Ph,Ak,H,[*1]

G5:O,S

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom 20:CLASS 21:CLASS
22:CLASS 24:CLASS 26:CLASS 27:CLASS 28:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 42:CLASS 43:CLASS 44:CLASS



chain nodes :

17 19 20 22 23 24 26 28 29 30 33 34 35 36 37

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21 38 39 40 41 42

chain bonds :

1-23 4-17 6-19 7-36 7-35 8-20 9-22 10-33 14-34 21-26 23-24 23-28 24-37 29-30

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
15-16 38-39 38-42 39-40 40-41 41-42

exact/norm bonds :

1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21
9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37
29-30 38-39 38-42 39-40 40-41 41-42

G1:O,S

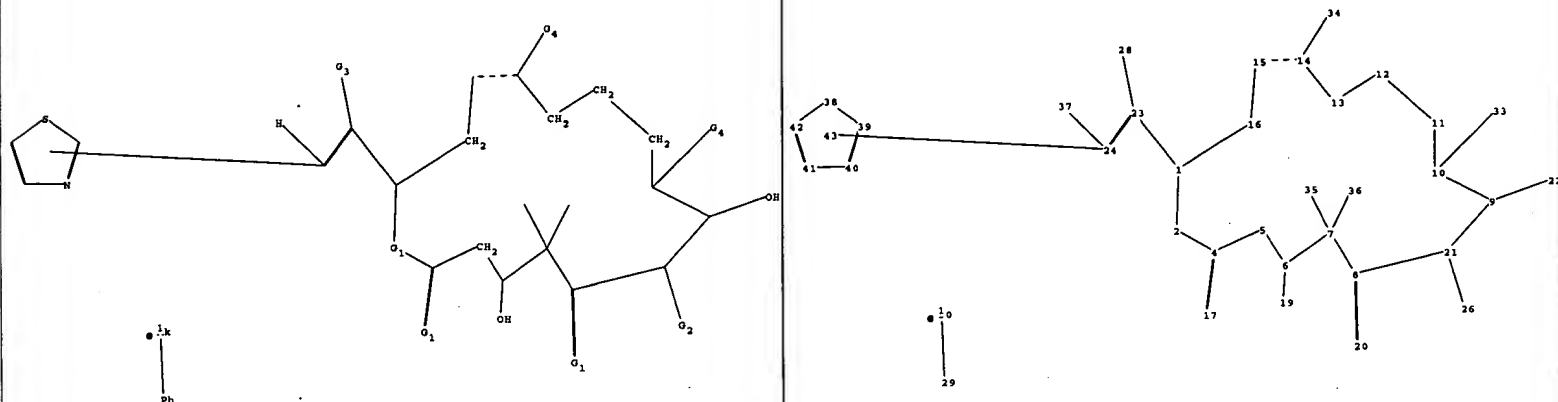
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-BU

G3:H,Ak

G4:Ph,Ak,H,[*1]

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS



chain nodes :

17 19 20 22 23 24 26 28 29 30 33 34 35 36 37

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21 38 39 40 41 42

chain bonds :

1-23 4-17 6-19 7-36 7-35 8-20 9-22 10-33 14-34 21-26 23-24 23-28 24-37 29-30

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
15-16 38-39 38-42 39-40 40-41 41-42

exact/norm bonds :

1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21
9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37
29-30 38-39 38-42 39-40 40-41 41-42

G1:O,S

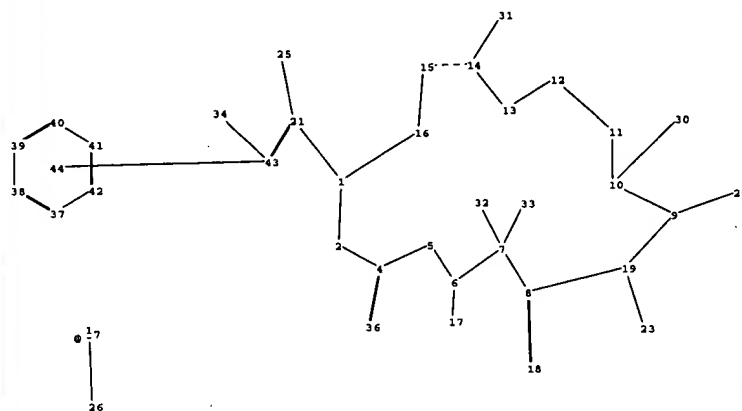
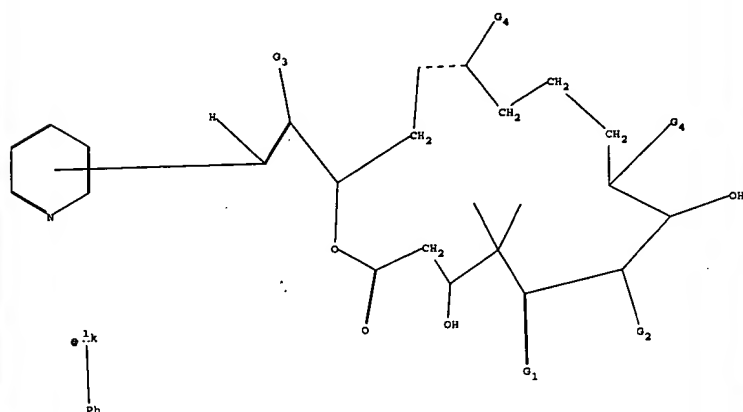
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

G4:Ph,Ak,H,[*1]

Match level :

1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS



chain nodes :

17 18 20 21 23 25 26 27 30 31 32 33 34 36 43

ring nodes :

1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 19 37 38 39 40 41 42

chain bonds :

1-21 4-36 6-17 7-33 7-32 8-18 9-20 10-30 14-31 19-23 21-25 21-43 26-27 34-43

ring bonds :

1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-19 9-10 9-19 10-11 11-12 12-13 13-14 14-15
15-16 37-38 37-42 38-39 39-40 40-41 41-42

exact/norm bonds :

1-2 1-16 2-4 4-5 4-36 5-6 6-7 6-17 7-8 8-18 8-19 9-10 9-19 9-20 10-11 10-30
11-12 12-13 13-14 14-15 14-31 15-16 19-23 21-25 26-27

exact bonds :

1-21 7-33 7-32 21-43 34-43

normalized bonds :

37-38 37-42 38-39 39-40 40-41 41-42

G1:O,S

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

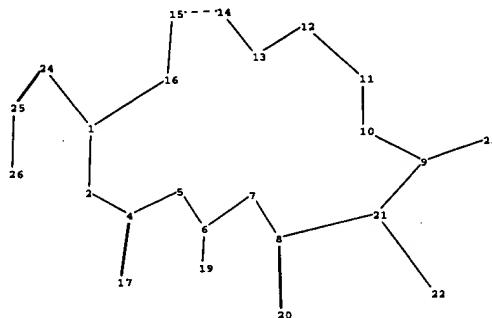
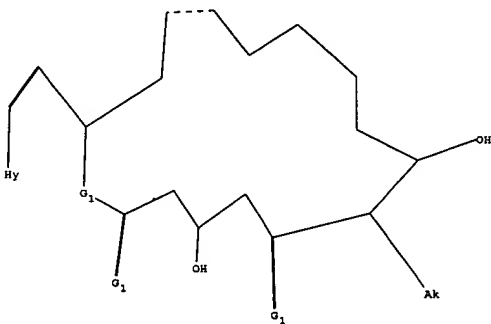
G3:H,Ak

G4:Ph,Ak,H,[*1]

G5:O,S

Match level :

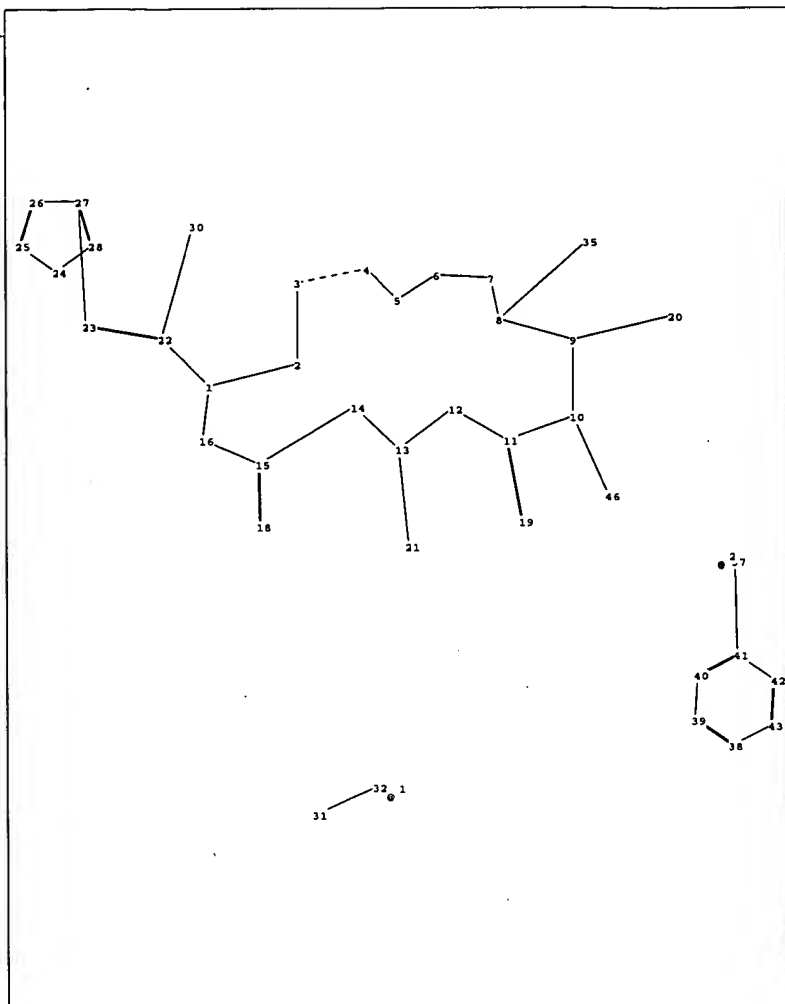
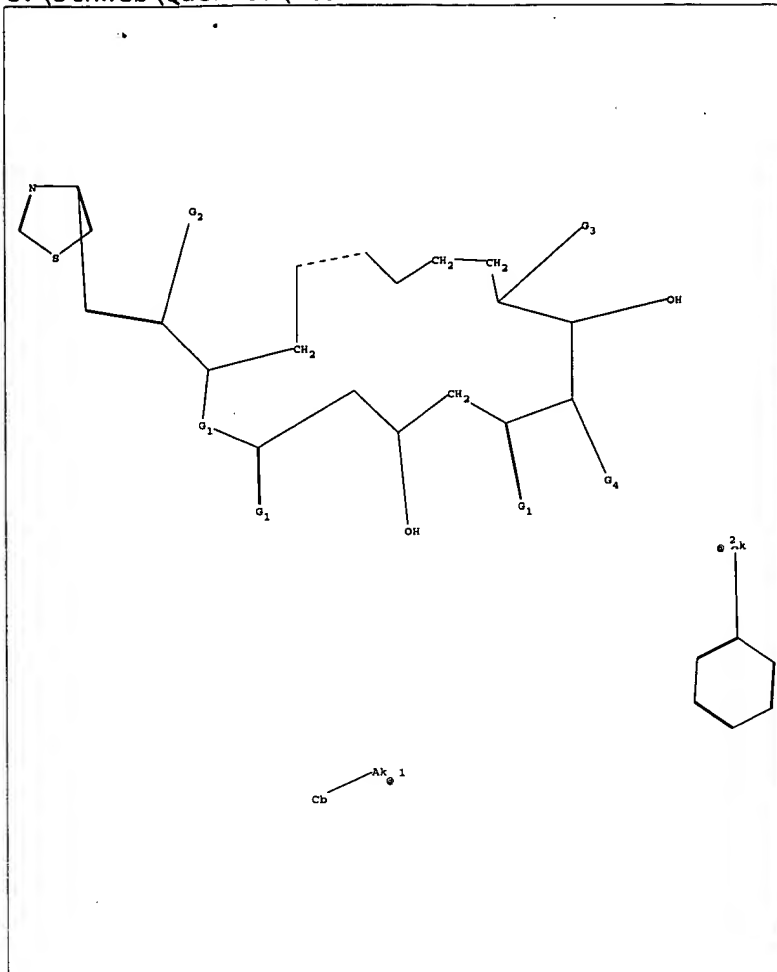
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom 20:CLASS 21:CLASS
23:CLASS 25:CLASS 26:CLASS 27:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:CLASS 43:CLASS 44:CLASS



chain nodes :
17 19 20 22 23 24 25 26
ring nodes :
1 2 4 5 6 7 8 9 10 11 12 13 14 15 16 21
chain bonds :
1-24 4-17 6-19 8-20 9-23 21-22 24-25 25-26
ring bonds :
1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
15-16
exact/norm bonds :
1-2 1-16 1-24 2-4 4-5 4-17 5-6 6-7 6-19 7-8 8-20 8-21 9-10 9-21 9-23 10-11
11-12 12-13 13-14 14-15 15-16 21-22 24-25 25-26

G1:O,S

Match level :
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS
24:CLASS 25:CLASS 26:Atom



chain nodes :

18 19 20 21 22 23 30 31 32 35 37 46

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 24 25 26 27 28 38 39 40 41
42 43

chain bonds :

1-22 8-35 9-20 10-46 11-19 13-21 15-18 22-23 22-30 23-27 31-32 37-41

ring bonds :

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
15-16 24-25 24-28 25-26 26-27 27-28 38-39 38-43 39-40 40-41 41-42 42-43

exact/norm bonds :

1-2 1-16 1-22 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 10-46 11-12
11-19 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26
26-27 27-28 31-32 37-41

normalized bonds :

38-39 38-43 39-40 40-41 41-42 42-43

isolated ring systems :

containing 24 :

G1:O,S

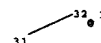
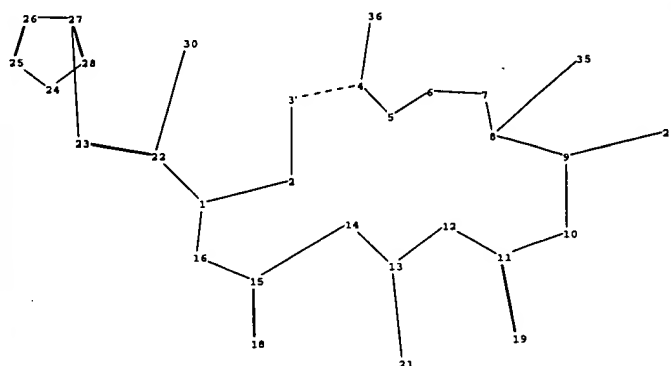
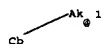
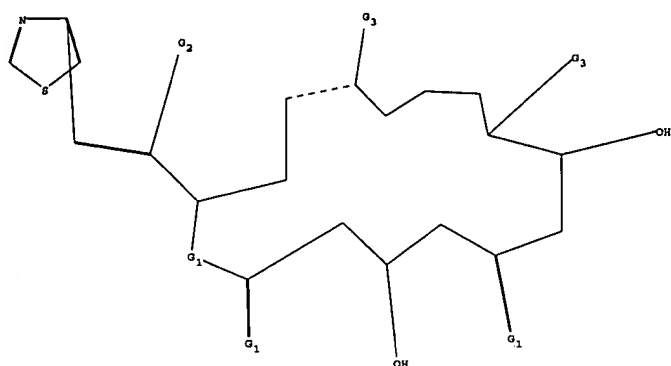
G2:H,Ak

G3:H,Cb,Ak,[*1]

G4:Ak,[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS
35:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 46:CLASS



chain nodes :

18 19 20 21 22 23 30 31 32 35 36

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 24 25 26 27 28

chain bonds :

1-22 4-36 8-35 9-20 11-19 13-21 15-18 22-23 22-30 23-27 31-32

ring bonds :

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
15-16 24-25 24-28 25-26 26-27 27-28

exact/norm bonds :

1-2 1-16 1-22 2-3 3-4 4-5 4-36 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 11-12
11-19 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26
26-27 27-28 31-32

isolated ring systems :

containing 24 :

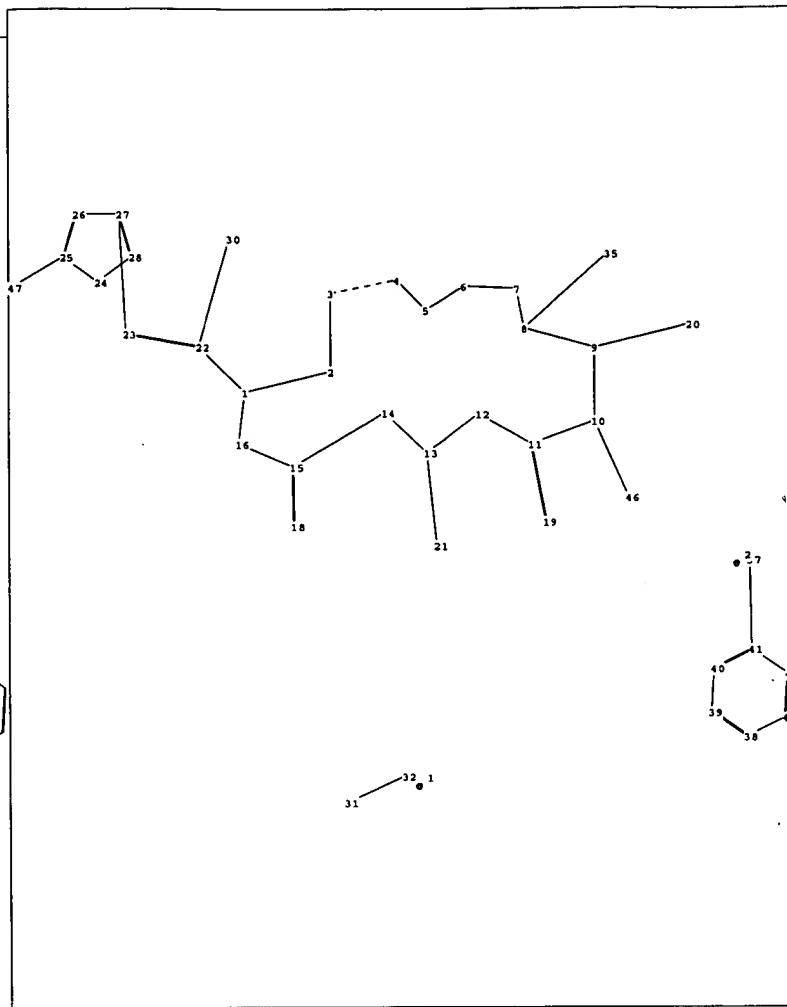
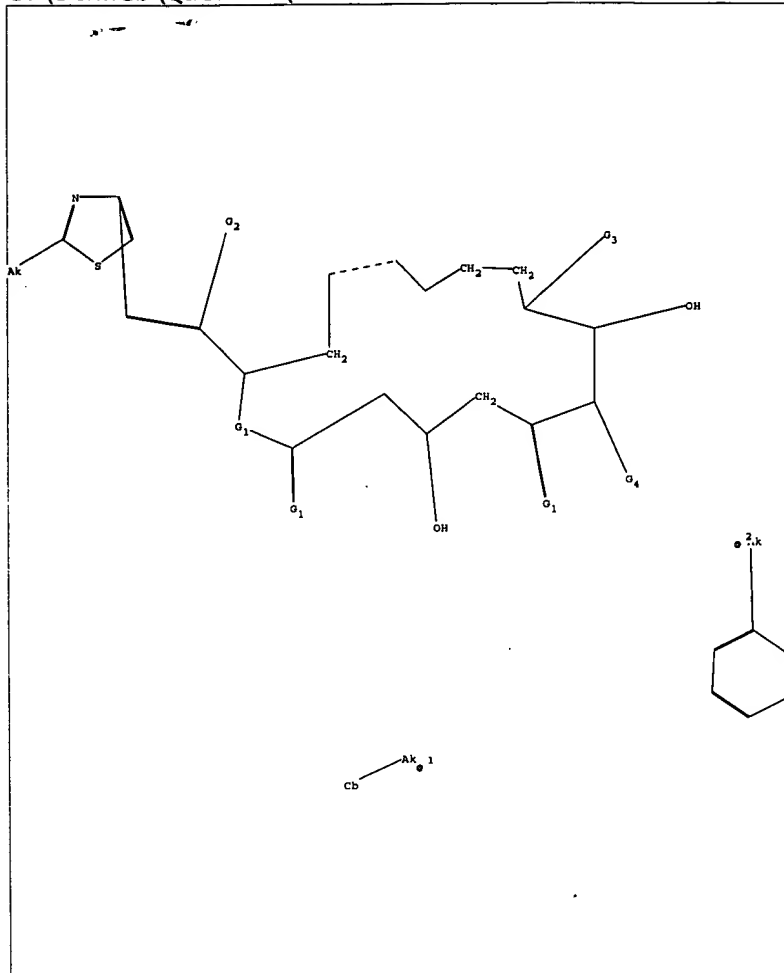
G1:O,S

G2:H,Ak

G3:H,Cb,Ak,[*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS
35:CLASS 36:CLASS



chain nodes :

18 19 20 21 22 23 30 31 32 35 37 46 47

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 24 25 26 27 28 38 39 40 41
42 43

chain bonds :

1-22 8-35 9-20 10-46 11-19 13-21 15-18 22-23 22-30 23-27 25-47 31-32 37-41

ring bonds :

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
15-16 24-25 24-28 25-26 26-27 27-28 38-39 38-43 39-40 40-41 41-42 42-43

exact/norm bonds :

1-2 1-16 1-22 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 10-46 11-12
11-19 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26
25-47 26-27 27-28 31-32 37-41

normalized bonds :

38-39 38-43 39-40 40-41 41-42 42-43

isolated ring systems :

containing 24 :

G1:O,S

G2:H,Ak

G3:H,Cb,Ak,[*1]

G4:Ak,[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS
35:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 46:CLASS
47:CLASS